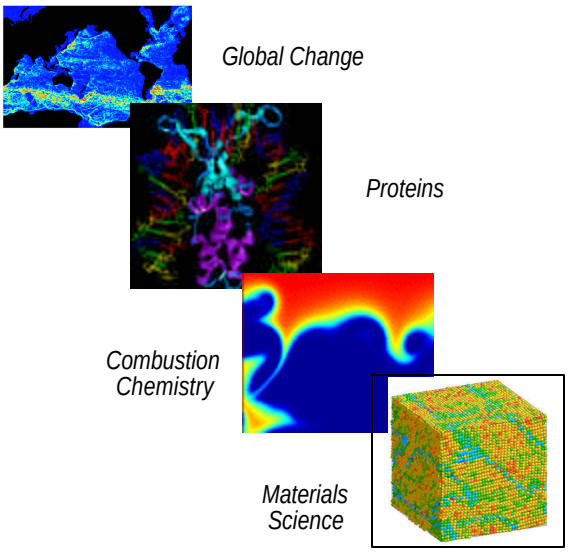
Office of Science

Advanced Scientific Computing Research

"Scientific Discovery through Advanced Computing"

http://www.sc.doe.gov/production/octr/index.html

Advanced scientific computing will be a key contributor to scientific research in the 21st Century. Within the Office of Science (SC), scientific computing programs and facilities are already essential to progress in many areas of research critical to the nation. Major scientific challenges exist in all SC research programs that can be addressed through advances in scientific supercomputing – designing materials atom-by- atom, revealing the functions of proteins, understanding and controlling plasma turbulence, designing new particle accelerators, and modeling global climate change, to name just a few.

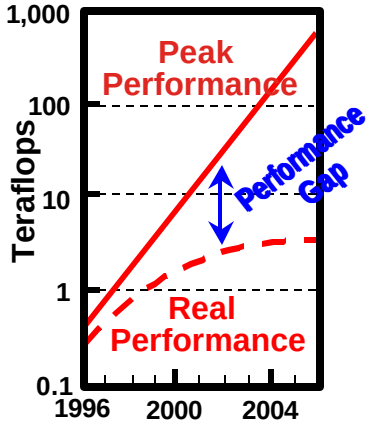


The Opportunity:

Today's computers are 100 times faster than the computers of a decade ago. In the next five to ten years, the largest scientific computers will be 1,000 times faster than today's. Using such computers, it will be possible to dramatically extend our exploration of the fundamental processes of nature as well as advance our ability to predict the behavior of a broad range of complex natural and engineered systems.

The Challenge:

To exploit this opportunity, these computing advances must be translated into corresponding increases in the performance of the scientific codes used to model physical, chemical, and biological systems. This is a daunting problem. Current advances in computing technology are being driven by market forces in the commercial sector, not by scientific computing. Harnessing commercial computing technology for scientific research poses problems never before encountered in supercomputing, in magnitude as well as in kind. This problem will only be solved by increasing investments in *computer software* – in research and development on scientific modeling codes, as well as on the mathematical and computing systems software that underlie these codes.



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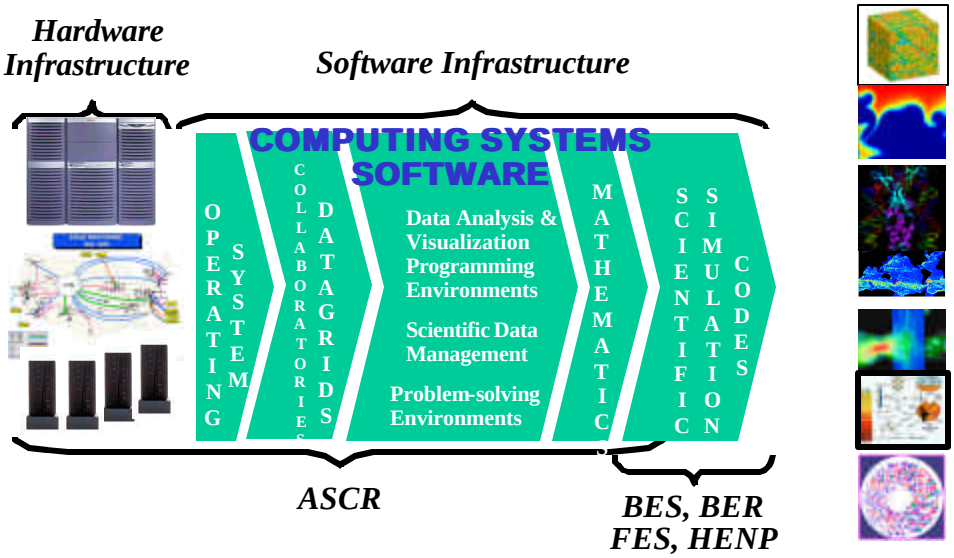
FY 2002 Investment Plan: In FY 2002 SC will continue the set of coordinated investments, which were competitively selected in FY 2001, focused on creating a *Scientific Computing Software Infrastructure* that bridges the gap between advanced computing technologies and its scientific research programs. The SC effort will:

- Create a new generation of *Scientific Challenge Codes* for terascale computers that can address the most critical scientific problems in SC's research programs.
- Create the *Mathematical and Computing Systems Software* to enable the Scientific Challenge Codes to take full advantage of the extraordinary capabilities of terascale computers.
- Create the *Collaboratory Software Infrastructure* to enable geographically-separated scientists to effectively work together as a team as well as provide electronic access to both facilities and data.

To initiate this effort, the Office of Science issued six grant solicitation notices (http://www.sc.doe.gov/production/grants/grants.html) with a combined value of $53 million. In response to these notices, more than 160 preproposals were received by mid-February, 2001. The magnitude of the response shows the interest this program has generated in the computational and scientific community.



The Benefits: The *Scientific Computing Software Infrastructure*, along with the upgrades to the hardware infrastructure, will enable laboratory and university researchers supported by the Office of Science to solve the most challenging scientific problems at a level of accuracy and detail never before achieved. These developments will have significant benefit to all of the government agencies which rely on high-performance scientific computing to achieve their mission goals as well as to the U.S. high-performance computing industry.